IUCLID 5
Guidance and support

Installation Guide for IUCLID 5 Version 5.3
Client-Server Architecture

Microsoft® Windows®

February 2011

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Table of Contents

1. Introduction 1
1.1. Hardware requirements 1
1.2. Software requirements 1
2. Making a fresh installation of IUCLID 5 3
2.1. Operating System 3
2.2. JAVA Development Kit 3
2.3. Installation of PostgreSQL 3
2.4. Configuration of PostgreSQL 7
2.5. Installation of a Web Application Server 13
2.5.1. Tomcat 13
2.6. Download IUCLID 5 15
2.7. Deployment in Tomcat 15
2.8. Changing the database connection settings 16
3. Upgrade 18
3.1. Upgrading from IUCLID 5.2 to IUCLID 5.3 for client-server architecture 18
3.1.1. Examples of the upgrade and migration processes per type of web application server 18
3.1.2. Starting IUCLID 5 after migration using the server method 21
3.2. Upgrading from IUCLID 5.0 or 5.1 to IUCLID 5.3 21
3.2.1. Migration of data to IUCLID 5.3 from IUCLID 5.0 or 5.1 21
3.2.2. Database configuration for running IUCLID 5.3 and a previous version at the same time 21
4. Initialisation of an installation of IUCLID 5 23
4.1. Starting IUCLID 5 23
4.2. First steps wizard 24
4.3. User management 30
5. Un-installation of IUCLID 5 31

Chapter 1. Introduction

IUCLID 5 can be installed as standalone or in a multi-user environment. This document describes how to install and configure the IUCLID 5 application in a distributed Microsoft® Windows® environment.

IUCLID 5 can be installed with the following open source components:

- JDK 1.6 or higher. Installation packages can be downloaded from http://www.java.com.
- Tomcat 5.5.x or 6.0.x (where x is the latest version). Installation packages can be downloaded from http://tomcat.apache.org
- PostgreSQL 8.2, 8.3 or 8.4 (recommended), but not 9. Do not use PostgreSQL 9. Installation packages can be downloaded from http://www.postgresql.org

For a IUCLID 5 installation using commercial software, the following components can be used:

- JDK 1.6 or higher. Installation packages can be downloaded from http://www.java.com.
- BEA WebLogic Server 9.0. http://www.oracle.com/bea
- Oracle® 10g or higher. Installation packages can be downloaded from http://www.oracle.com

  The Oracle driver for Java is no longer supplied with the IUCLID installation package. The correct driver for the combination of Java and Oracle versions in use must be obtained from the oracle web site and installed in the appropriate folder. For example, for Java 1.6 and Oracle 11g Release 2 (11.2.0.2.0), the name of the driver is `ojdbc6.jar`. For use with Tomcat, the driver must be placed in Tomcat's library folder, e.g. `Tomcat\lib`.

If you encounter any problems during the installation that cannot be solved using information in this manual, or the documentation of third party softwares; before contacting the ECHA Helpdesk, please try the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.

1.1. Hardware requirements

The server hosting IUCLID 5 must have at least:

- RAM: 1 GB (recommended 2 GB)
- Hard disk space: 200 GB
- CPU: 2 GHz, 32 or 64 bit architecture
- Network adapter 100 Mbps (recommended 1Gbps)

The requirements depend in part on the plugins that are in use. For example, using the Query Tool plugin will increase the resources required to obtain a reasonable running speed; especially on a large database.

1.2. Software requirements

In addition to either one of the groups of software components stated above, for commercial or open source, the following are required:

- Windows 2003 Server. For installation instructions, please refer to the documentation of the manufacturer.
- The IUCLID 5 distributed installation package, version 5.3. It can be downloaded without charge from the IUCLID 5 web site.
- Once you have completed the installation of IUCLID 5, you should test it by starting and configuring it. The configuration requires access to at least a legal entity file (LEOX). The creation of a LEOX is described on the IUCLID 5 web site where the

installation software is published. In addition, it is recommended to upload a set of reference substances and the EC inventory. These are also available from the web site at which the IUCLID 5 software is published.

Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set*, a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

For more information regarding system requirements, see the FAQ on the IUCLID web site located at http://iuclid.eu.

Chapter 2. Making a fresh installation of IUCLID 5

The following chapter contains a brief description of the actions required to make a fresh installation of IUCLID 5 that runs within a web server on Windows.

2.1. Operating System

IUCLID 5 has been tested thoroughly using Windows server 2003. Other versions (2000, XP, 2008) may be used as well. In that case the file locations might be different from the ones used in this document. For installation instructions, please refer to the documentation of the manufacturer.

2.2. JAVA Development Kit

Download the JAVA Development Kit (JDK) 6 or JAVA Runtime Environment (JRE) 6 according to the architecture of your computer from http://java.sun.com/javase/downloads/index.jsp. Select the latest available update.

Run the installer and follow the instructions. The default parameters are appropriate for IUCLID 5. For more information please refer to the installation instructions http://java.sun.com/javase/6/webnotes/install/index.html.

2.3. Installation of PostgreSQL

If PostgreSQL 8.2, 8.3 or 8.4 are not already installed on the computer, download 8.4 from the site www.postgresql.org/download and install it. Do not use PostgreSQL 9. The web site of PostgreSQL offers a range of alternative ways to download and install the PostgreSQL software. The screen shots shown below show the use of the *one click installer* available from the PostgreSQL web site for PostgreSQL 8.4. An example of the file name of the installer is *postgresql-8.4.7-1-windows.exe*.

If version 8.2, 8.3 or 8.4 of PostgreSQL is already running as a service with a user `postgres`, the existing installation can be used, although the latest 8.4 is recommended. The default fresh installation of PostgreSQL 8.4, made using the *one click installer*, automatically starts PostgreSQL as a service, creates the user `postgres` if necessary, and supplies administration tools (e.g. pgAdmin III) that can be used to create the database. If the installer creates the superuser `postgres`, you will have to create a password for it, as shown in the figure below, and enter it later into the configuration file for IUCLID 5.

Figure 2.1. Installer for PostgreSQL version 8.4

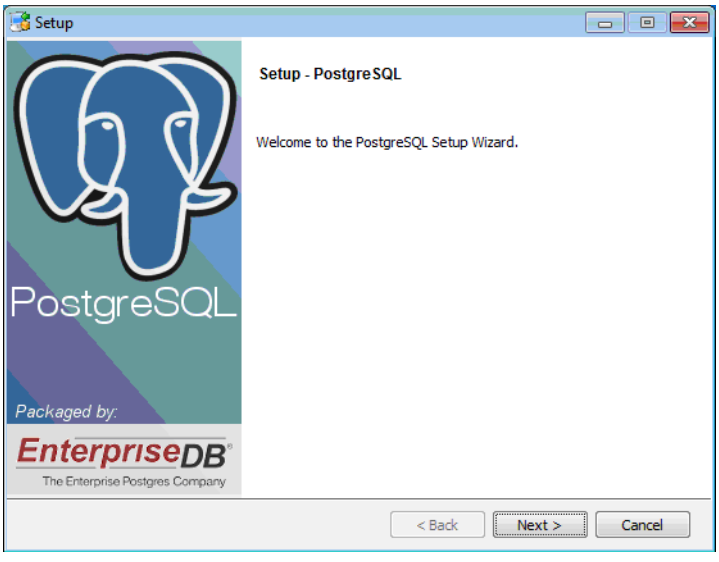


Figure 2.2. Installation directory for PostgreSQL

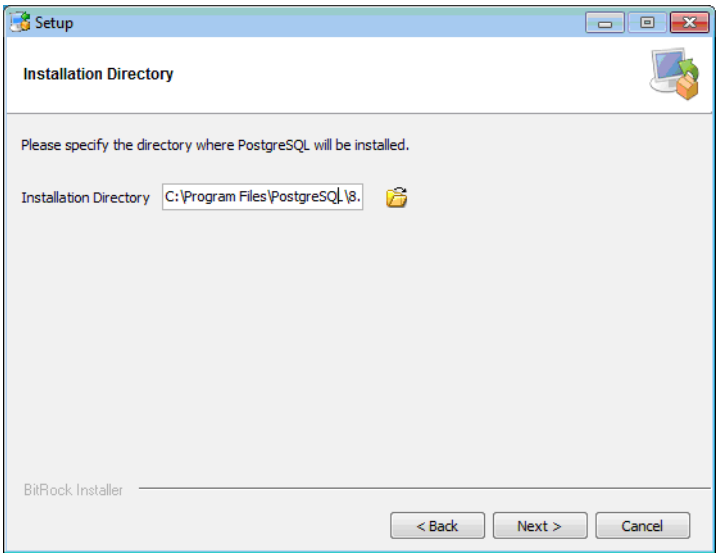


Figure 2.3. Data directory for PostgreSQL

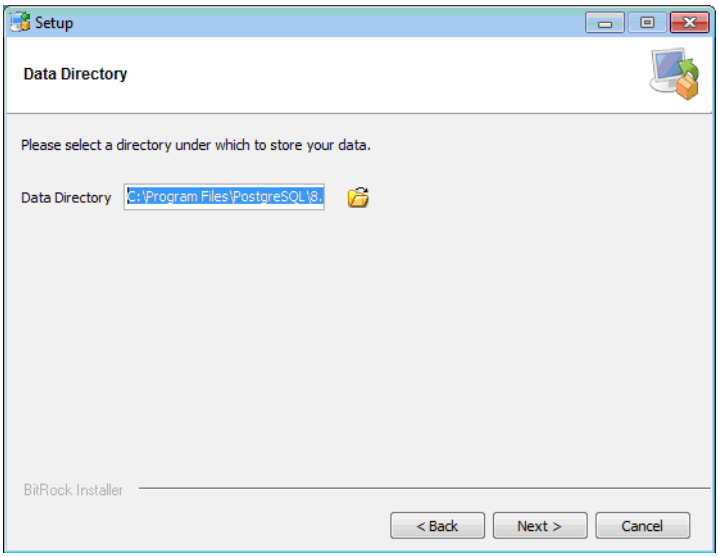


Figure 2.4. Password for the database superuser (postgres) and the Windows service account (postgres)

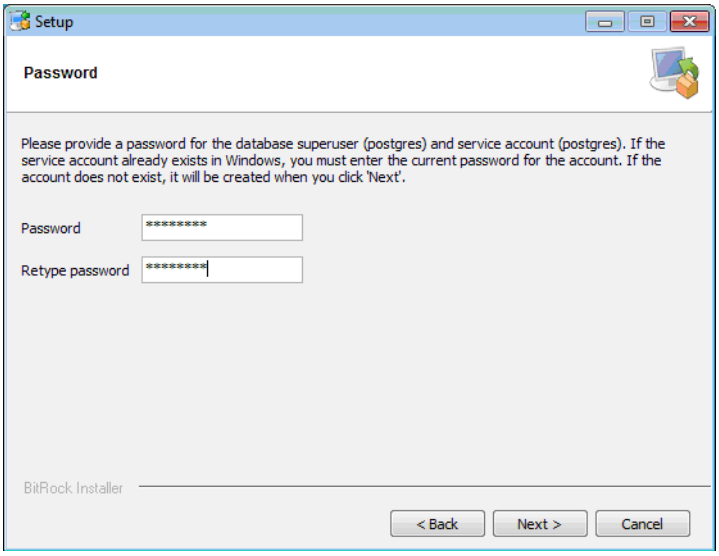

Setup
Password
Please provide a password for the database superuser (postgres) and service account (postgres). If the service account already exists in Windows, you must enter the current password for the account. If the account does not exist, it will be created when you click 'Next'.
Password
Retype password
BitRock Installer
< Back
Next >
Cancel

Figure 2.5. Port number for PostgreSQL

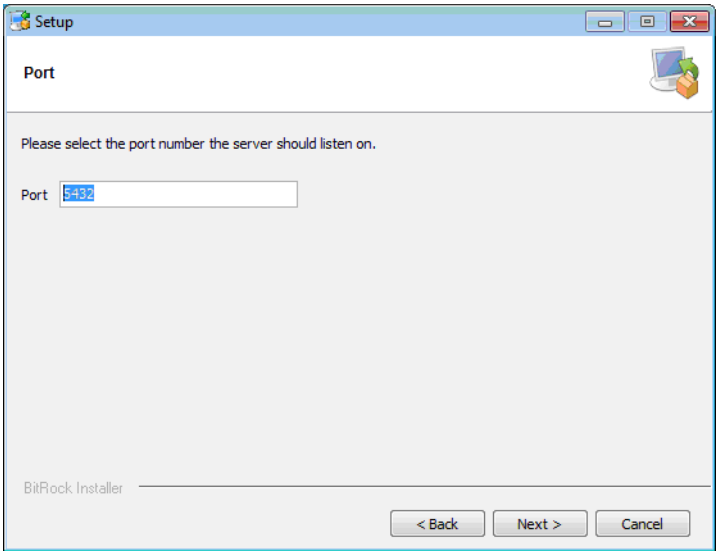


Figure 2.6. Set the default locale for PostgreSQL

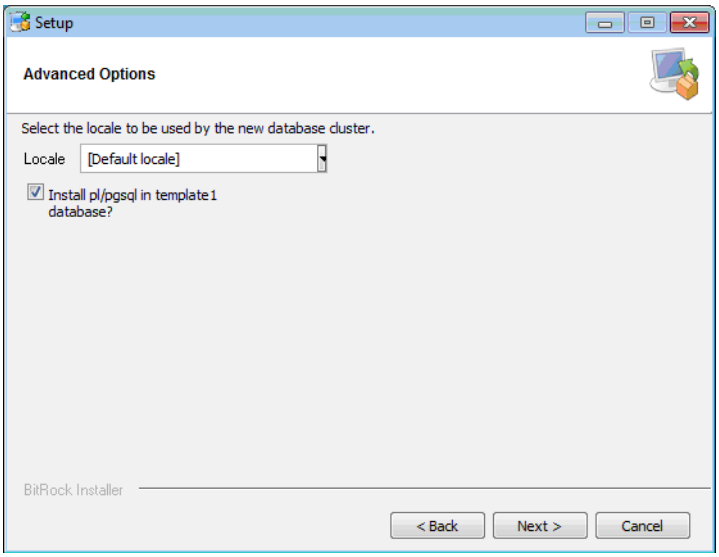


Figure 2.7. Confirm installation of PostgreSQL

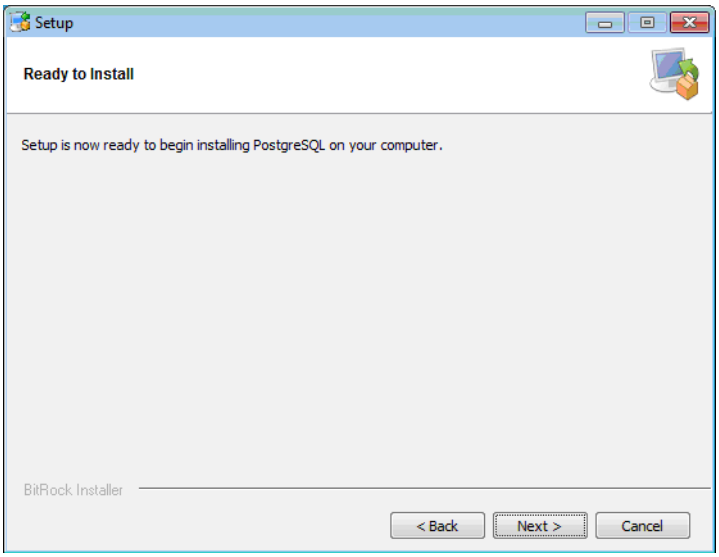


Figure 2.8. Installation of PostgreSQL in progress

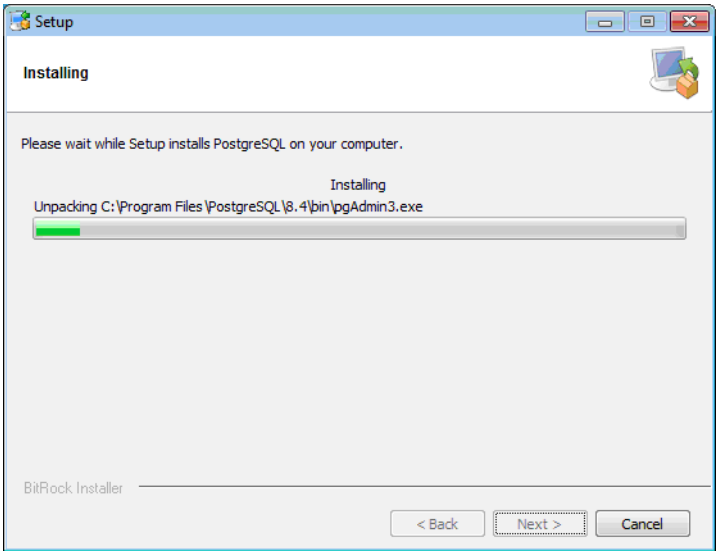
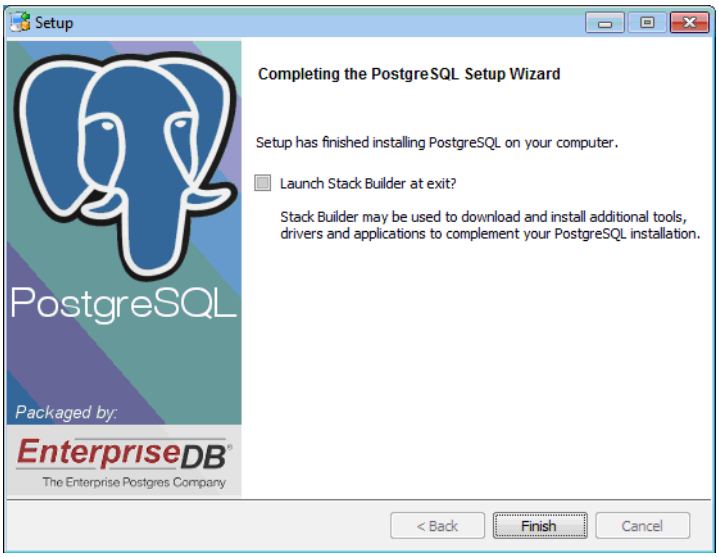


Figure 2.9. Installation of PostgreSQL complete


Setup
PostgreSQL
Packaged by:
EnterpriseDB
The Enterprise Postgres Company
Completing the PostgreSQL Setup Wizard
Setup has finished installing PostgreSQL on your computer.
Launch Stack Builder at exit?
Stack Builder may be used to download and install additional tools, drivers and applications to complement your PostgreSQL installation.
< Back
Finish
Cancel

2.4. Configuration of PostgreSQL

A new user and a new database need to be created.

Tip

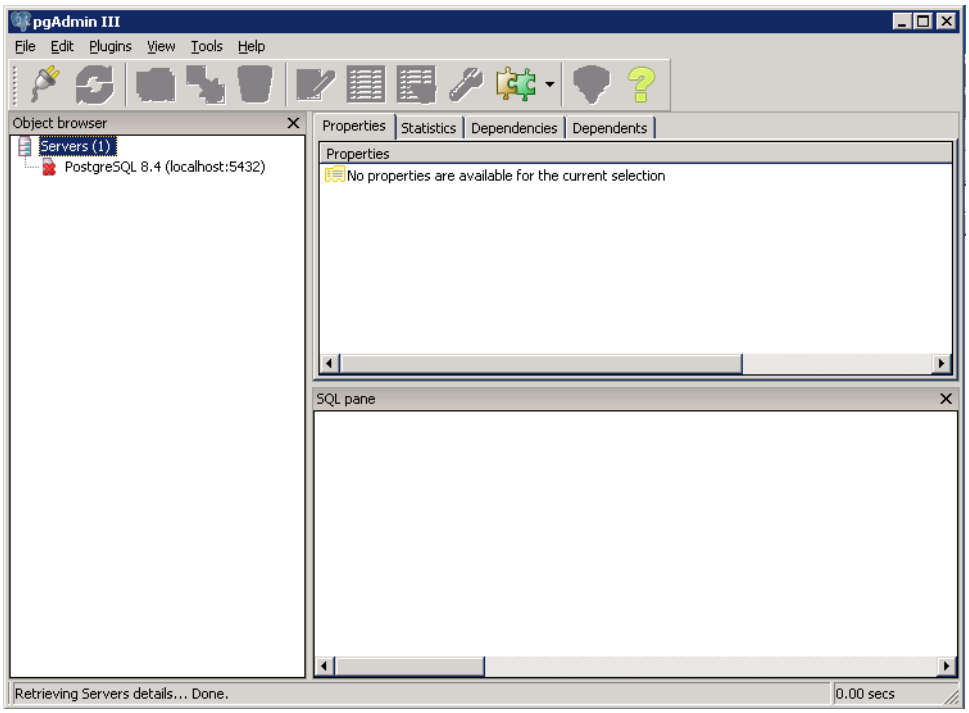
IUCLID 5 is configured by default to connect to the database using username:*iuclid5* and password:*iuclid5*. It is convenient to specify the same password now, and change it later when the application is set up correctly.

Important

Take note of the password of this user. This user name and password will be needed later to connect IUCLID 5 to the database.

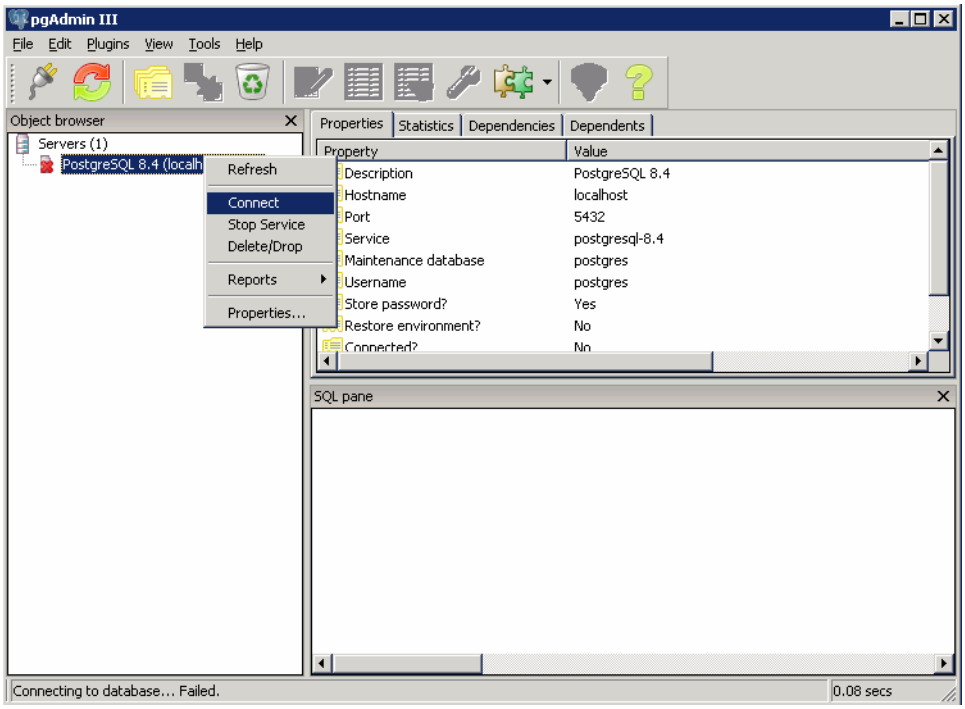
The program pgAdmin III can be used to create the database as follows. Start pgAdmin III from the menu *Start / All Programs / PostgreSQL 8.4*. After the splash screen has appeared and you have closed the pop-up window that shows usage tips, the following screen is shown.

Figure 2.10. pgAdmin III interface on first opening



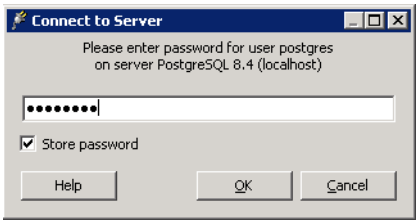
Right-click the text *PostgreSQL 8.4(localhost:5432)* that is under the word *Servers* highlighted in blue in the figure above. Select *connect* as shown below.

Figure 2.11. Connect pgAdmin III to PostgreSQL as user *postgres*



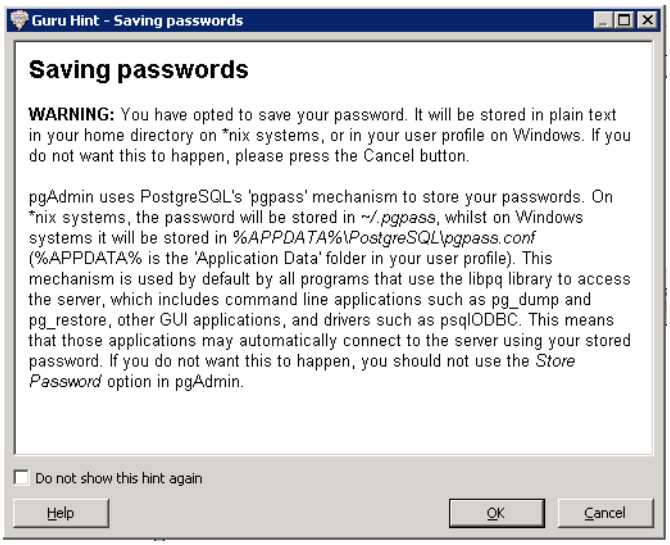
Enter the password for user *postgres* as given in the postgres installer Figure 2.4, “Password for the database superuser (postgres) and the Windows service account (postgres)” then click *OK*. It is recommended to store the password to facilitate future access.

Figure 2.12. Authenticate user *postgres*



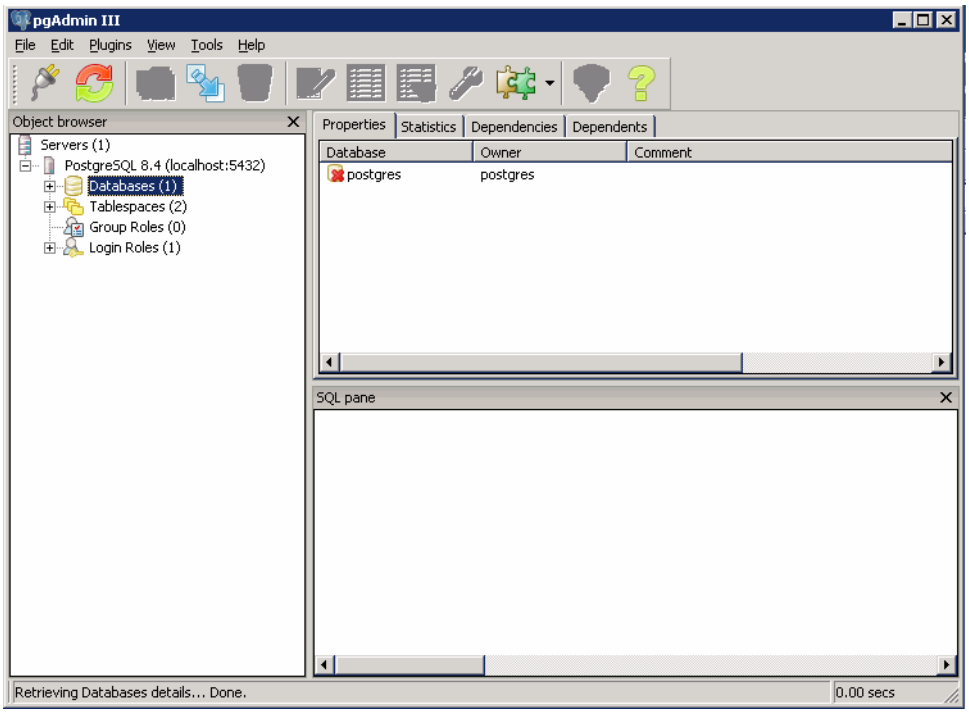
When you elect to save the password, the following warning may be displayed. Click *OK*

Figure 2.13. Saving passwords Warning


Guru Hint - Saving passwords
Saving passwords
WARNING: You have opted to save your password. It will be stored in plain text in your home directory on *nix systems, or in your user profile on Windows. If you do not want this to happen, please press the Cancel button.
pgAdmin uses PostgreSQL's 'pgpass' mechanism to store your passwords. On *nix systems, the password will be stored in ~/.pgpass, whilst on Windows systems it will be stored in %APPDATA%\PostgreSQL\pgpass.conf (%APPDATA% is the 'Application Data' folder in your user profile). This mechanism is used by default by all programs that use the libpq library to access the server, which includes command line applications such as pg_dump and pg_restore, other GUI applications, and drivers such as psqlODBC. This means that those applications may automatically connect to the server using your stored password. If you do not want this to happen, you should not use the Store Password option in pgAdmin.
Do not show this hint again
Help
OK
Cancel

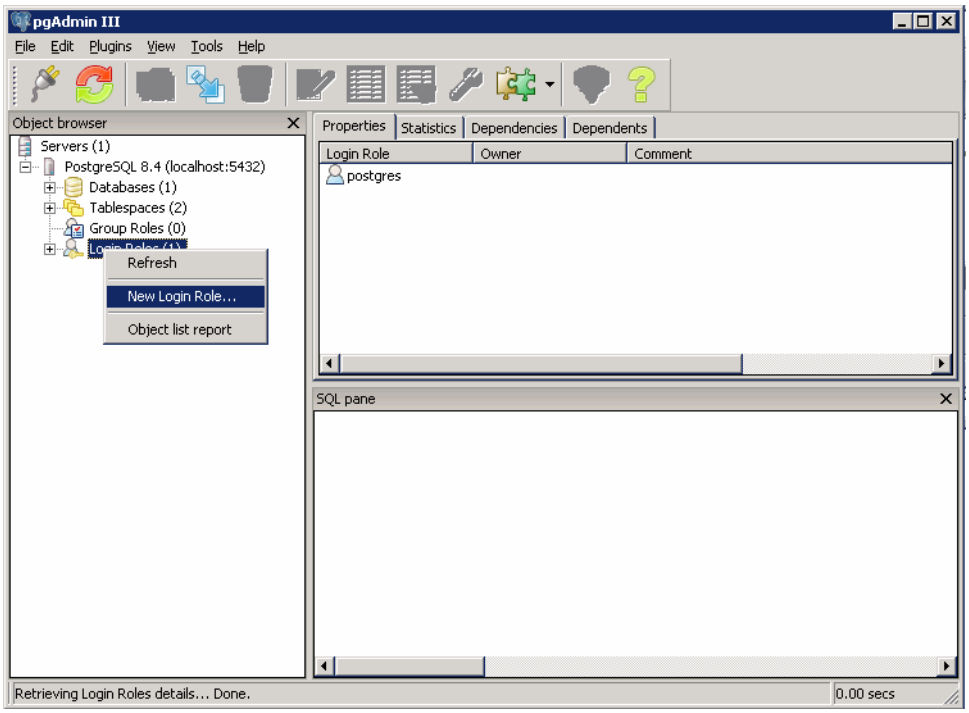
Expand the tree for *PostgreSQL 8.3(localhost:5432)* by clicking the plus sign that has just appeared next to it, as shown in the figure below.

Figure 2.14. Initial screen in pgAdmin III



Right-click on *Login Roles* and select *New Login Role...*.

Figure 2.15. Select create a new user option

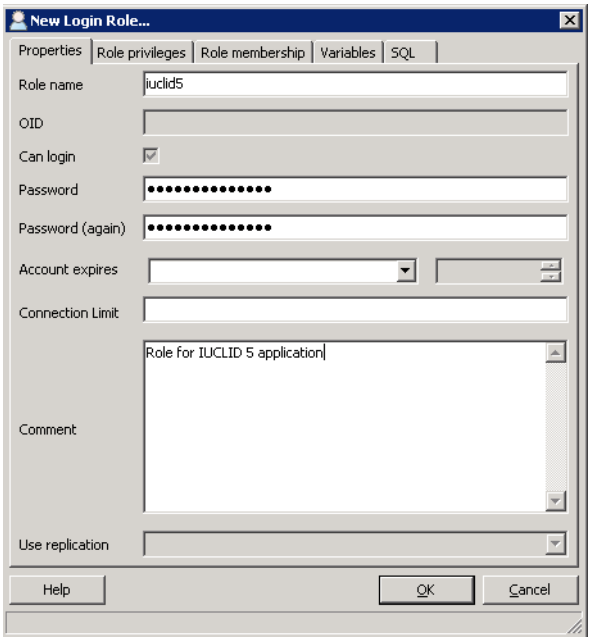


Enter the role name *iuclid5*. Set the password.

Important

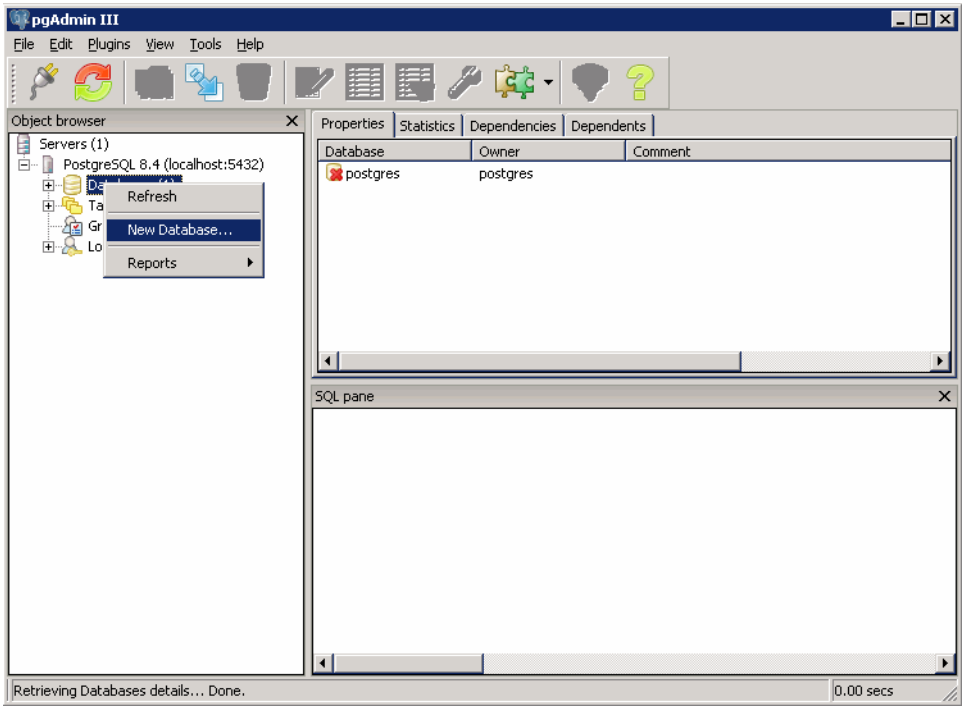
Make a note of the user name and password. They are referred to later in the installation, in section Section 2.8, “Changing the database connection settings”. We recommend using `iuclid5` as both the user name and the password.

Figure 2.16. Create new role (i.e. a user) with name 'iuclid5'



Request a new database by right-clicking the text *Databases* and selecting *New Database...* as shown in the figure below.

Figure 2.17. Request a new database in pgAdmin III

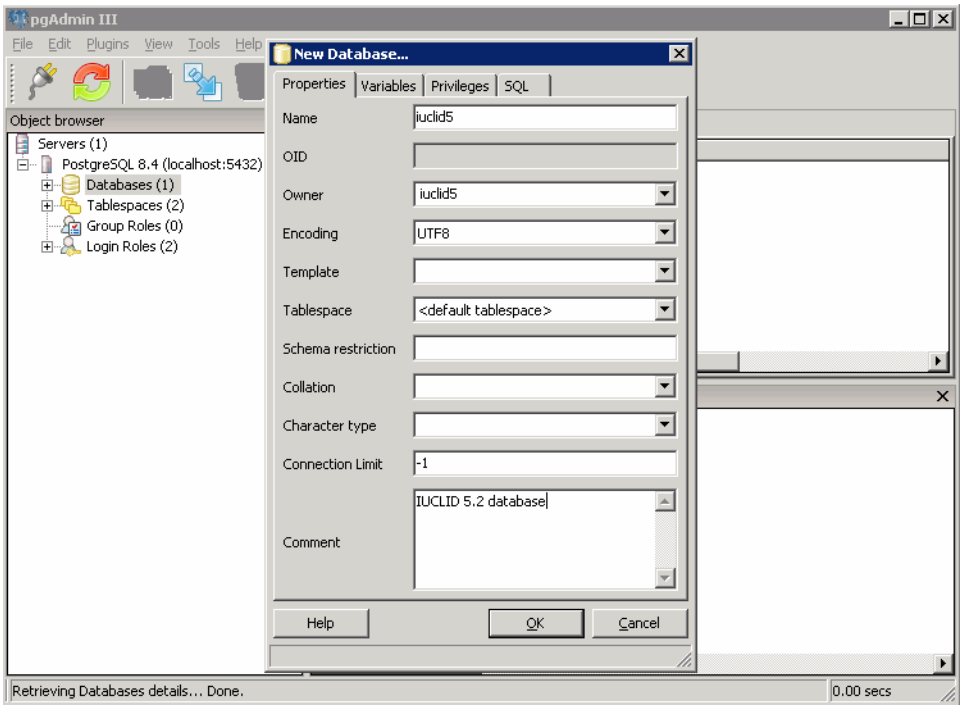


Enter the details you require. Normally these are only name=iuclid5 and owner=iuclid5. The encoding should be UTF8. Click *OK*.

Important

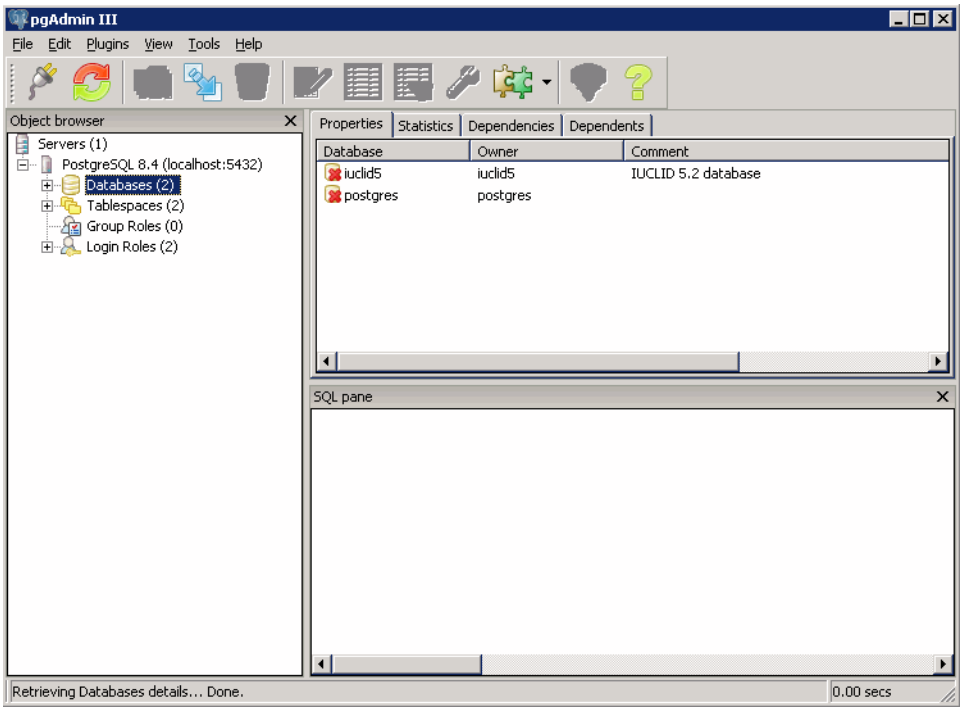
Make a note of the database name. It is referred to later in the installation, in section Section 2.8, “Changing the database connection settings”. We recommend using the name `iuclid5`.

Figure 2.18. Enter the details of IUCLID 5's database into pgAdmin III



As you can see from the figure below, there is now a new database named *iuclid5*.

Figure 2.19. List of databases in pgAdmin III



You can now close *pgAdmin III* and move directly to the installation of IUCLID 5.

2.5. Installation of a Web Application Server

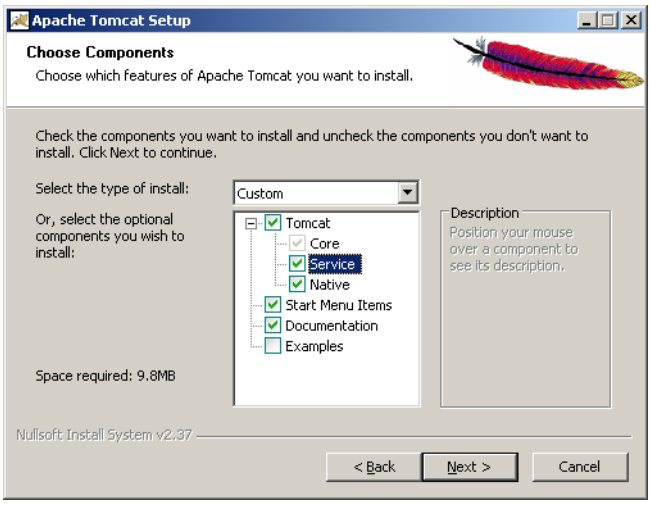
Here is described the installation of the Tomcat Web Application Server. BEA Web Logic can be used instead.

2.5.1. Tomcat

Download the Windows Service Installer of Tomcat 6.0 from http://tomcat.apache.org/.

At *Choose Components* step select also the *Service* and *Native* components.

Figure 2.20. Choose Components

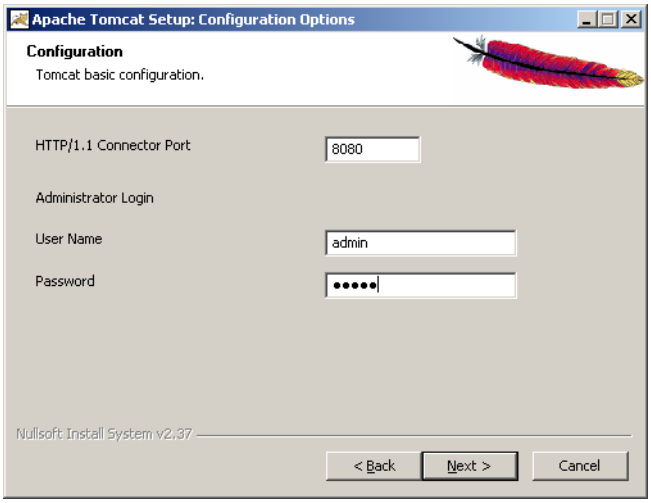

Apache Tomcat Setup
Choose Components
Choose which features of Apache Tomcat you want to install.
Check the components you want to install and uncheck the components you don't want to install. Click Next to continue.
Select the type of install:
Custom
Or, select the optional components you wish to install:
Tomcat
Core
Service
Native
Start Menu Items
Documentation
Examples
Description
Position your mouse over a component to see its description.
Space required: 9.8MB
Nullsoft Install System v2.37
< Back
Next >
Cancel

Type a name and password for the Tomcat administrator.

Important

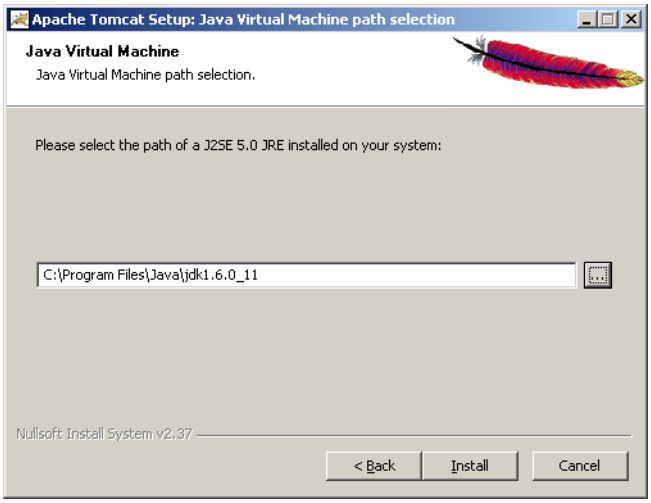
Take note of this settings because they are required to access the Tomcat Manager to deploy and remove applications.

Figure 2.21. Configuration



Select the folder of the previously installed Java Virtual Machine

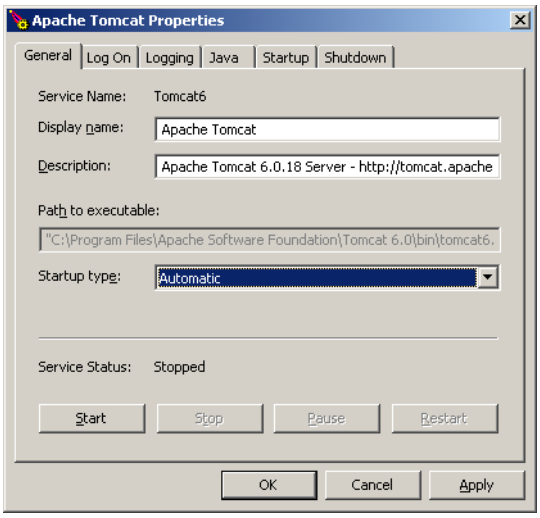
Figure 2.22. Java Virtual Machine


Apache Tomcat Setup: Java Virtual Machine path selection
Java Virtual Machine
Java Virtual Machine path selection.
Please select the path of a J2SE 5.0 JRE installed on your system:
C:\Program Files\Java\jdk1.6.0_11
Nullsoft Install System v2,37
< Back
Install
Cancel

When the installation process is finished a new icon appears in the system tray for Tomcat (right-bottom corner of your screen). Right-click on the icon and select Configure...

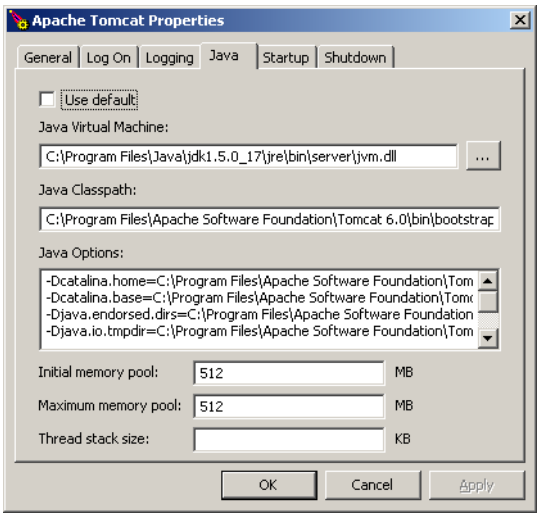
On the General tab set Automatic startup type.

Figure 2.23. General tab



On the Java tab type 512 MB for both Initial memory pool and Maximum memory pool.

Figure 2.24. Java tab



Restart the service by right-clicking on the tray icon and selecting Stop Service then Start Service.

Open the page http://localhost:8080/manager/html/ in your browser, enter the username and password you gave to the Tomcat administrator and check the memory settings currently set for Tomcat. The Max memory in the JVM section of the Server Status page should be at least 500 MB.

2.6. Download IUCLID 5

Before downloading IUCLID 5 you need to register as a IUCLID user on the IUCLID website [http://iuclid.eu/]. The application itself is packaged into the `iuclid5_server.zip` file.

2.7. Deployment in Tomcat

Deployment is the term used for the process of installing a web application into the Tomcat server.

Web application deployment may be accomplished in two ways.

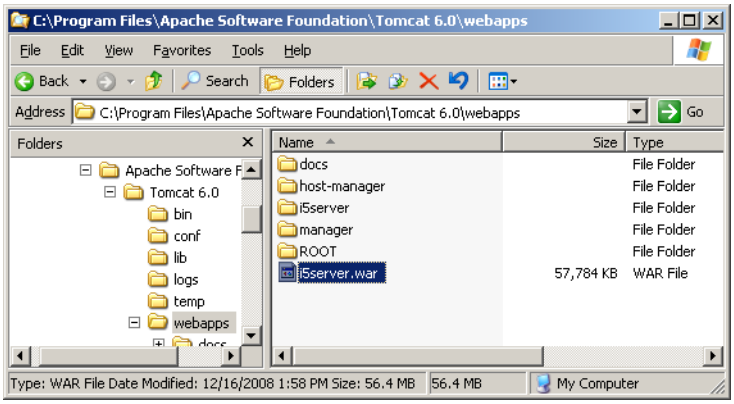
- Statically - the web application is set up before Tomcat is started
- Dynamically - in conjunction with the Tomcat Manager web application or manipulating already deployed web applications

You can find more information about how to deploy a web application on tomcat on the Tomcat deployment [http://tomcat.apache.org/tomcat-5.5-doc/deployer-howto.html] web page.

In this document only the Dynamic deployment is described. However also the static deployment may be used.

The deployment of IUCLID 5 actually consists of copying the `i5server.war` archive into the `webapps` directory of Tomcat.

Figure 2.25. IUCLID 5 Deployment



Note

When IUCLID 5 is started the first time it creates new tables in the database which might take up to 30 seconds.

2.8. Changing the database connection settings

If the username, password and name of the database are all *iuclid5*, the application will start normally, otherwise it cannot connect to the database and the database settings have to be adjusted.

Open the `server.properties` file in the `webapps/i5server/WEB-INF/classes directory.`

The `server.properties` file is the configuration of the IUCLID 5 server. In order to connect to the database correctly it is necessary to modify the `server.properties` configuration file. The default configuration file contains settings in order to connect to a PostgreSQL database on the same computer. Usually it is sufficient to specify the database password.

```
#
# Settings for using PostgreSQL
#
hibernate.connection.url=jdbc:postgresql://localhost:5432/iuclid5
hibernate.connection.username=iuclid5
hibernate.connection.password=iuclid5
hibernate.connection.driver_class=org.postgresql.Driver
hibernate.dialect=org.hibernate.dialect.PostgreSQLDialect
```

If your database server is running on another computer or database name, or the username is different, modify the settings accordingly. For example, if your database server's name is dbserver, PostgreSQL is accepting connections on port 12345, the database name is chemdb and the user is joe with password xxxx, your configuration is:

```
hibernate.connection.url=jdbc:postgresql://dbserver:12345/chemdb
hibernate.connection.username=joe
hibernate.connection.password=xxxx
```

Important

Make sure that there are no spaces after the username and password values in the properties file.

The IUCLID 5 server registers the activities into a log file which helps the system administrator. The configuration file for setting the logging is `i5server.logging.properties` in the `WEB-INF/classes` directory.

Start Tomcat using the Tomcat server icon.

All the software has now been installed. What remains, is some configuration, as described in the next section.

Chapter 3. Upgrade

This chapter describes how to upgrade a previous version of IUCLID 5 to IUCLID 5.3. Dependent upon the version of IUCLID 5 that is being upgraded to IUCLID 5.3, there are two main scenarios in the upgrade process. One is to upgrade from any version 5.2, whereas the other is to upgrade from 5.0 or 5.1. These are each described in a dedicated sub-section of this chapter. In all scenarios, before starting the upgrade, it is important to back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up functionality of the database. Making only a copy of the file system on which IUCLID is installed is not recommended as a means of backing-up.

3.1. Upgrading from IUCLID 5.2 to IUCLID 5.3 for client-server architecture

This section is relevant only if the upgrade is from IUCLID 5.2. For earlier versions, see the next section. The version can be seen from within the interface of IUCLID 5. To see the version, start IUCLID 5, log-in, then click *Help* and select *About*. The upgrade process can be summarised by the steps shown below. Detailed step by step examples are given in following subsections:

1. Back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up function of the database software, for example PostgreSQL.
2. Remove the executable program files for the previous version of IUCLID. Note that the plugins for IUCLID 5.2.x are not compatible with IUCLID 5.3. Therefore, they must not be copied over to the new installation.
3. Copy the executable program files for the new version of IUCLID to the installation destination
4. Adapt the configuration files for IUCLID if necessary. Note that if the Oracle database is used, the file `server.properties` must contain the following entry:

   ```
   hibernate.connection.driver_class=oracle.jdbc.OracleDriver
   ```

   The previous value was:

   ```
   hibernate.connection.driver_class=oracle.jdbc.driver.OracleDriver
   ```

5. Migrate the database by running IUCLID in update mode only once. This is done as follows. First ensure the IUCLID web application is stopped. Uncomment the following line in the file `server.properties`:

   ```
   database.update.startup=true
   ```

   Start the application, wait for the migration to finish, then stop the application. Comment out the previously edited line in the file `server.properties`:

   ```
   #database.update.startup=true
   ```

6. Once the migration process has been completed successfully, the new version of IUCLID can be started and checked before being entered into production.

3.1.1. Examples of the upgrade and migration processes per type of web application server

The detailed actions required for step 2-5 above depend on the particular web application server in use. Examples are given below for the web application servers relevant to this document:

3.1.1.1. Upgrade and migrate from IUCLID 5.2 to IUCLID 5.3 under Tomcat

1. Close all clients for IUCLID 5.
2. Shutdown the IUCLID 5 server, for example by shutting down Tomcat
3. Copy the configuration file `server.properties` into a backup folder. For example:

   copy `%TOMCAT%\webapps\i5server\WEB-INF\classes\server.properties`

   to

   `e:\backup\server.properties`
4. Delete the folder with the old IUCLID 5 program. For example:

   rd `%TOMCAT%\webapps\i5server\`
5. Copy the file `i5server.war` into the folder `webapps`. For example:

   copy `i5server.war`

   to

   `%TOMCAT%\webapps`
6. Start Tomcat and it will automatically unpack and start the application. The content of the war file will be extracted to a folder. For example:

   `%TOMCAT%\webapps\i5server`
7. Shutdown Tomcat.
8. Copy the file `server.properties` from the backup folder into the folder `%TOMCAT%\webapps\i5server\WEB-INF\classes`. For example:

   copy `e:\backup\server.properties`

   to `%TOMCAT%\webapps\i5server\WEB-INF\classes\server.properties`
9. Note that if the Oracle database is to used, the file `server.properties` must contain the following entry:

   ```
   hibernate.connection.driver_class=oracle.jdbc.OracleDriver
   ```

   The previous value was:

   ```
   hibernate.connection.driver_class=oracle.jdbc.driver.OracleDriver
   ```
10. Set IUCLID 5 to start in its update mode by uncommenting the following line in the file `server.properties`

    ```
    database.update.startup=true
    ```
11. Start the IUCLID 5 server, by starting Tomcat, and wait until the IUCLID database has been migrated. This can be followed from logs. During the migration, the IUCLID server status is *Unavailable*.
12. Stop the IUCLID 5 server, by stopping Tomcat.
13. Set IUCLID 5 to start not in its update mode by commenting out the line edited in step (10):

```
#database.update.startup=true
```

14.Start the IUCLID 5 server, by starting Tomcat.

3.1.1.2. Upgrade and migrate from IUCLID 5.2 to IUCLID 5.3 under BEA WebLogic Server

1. Close all clients for IUCLID 5.
2. Shutdown the IUCLID 5 server, for example by shutting down BEA WebLogic Server
3. Copy the configuration file `server.properties` into a backup folder. For example:

   copy `c:\program files\IUCLID5\i5server\server.properties`

   to

   `e:\backup\server.properties`
4. Delete the folder with the old IUCLID 5 program. For example:

   rd `c:\program files\IUCLID5\i5server`
5. Copy the file `i5server.war` into the folder `%IUCLID5%`. For example:

   copy `i5server.war`

   to

   `c:\program files\IUCLID5\`
6. Create a folder:

   `mkdir i5server`
7. Move into the new folder:

   `cd i5server`
8. Unzip the WAR file to this folder:

   `unzip ..\i5server.war`
9. Copy the file `server.properties` from the backup folder into the folder `%TOMCAT%\webapps\i5server\WEB-INF\classes`. For example:

   copy `e:\backup\server.properties`

   to `%TOMCAT%\webapps\i5server\WEB-INF\classes\server.properties`
10. Note that if the Oracle database is to used, the file `server.properties` must contain the following entry:

```
hibernate.connection.driver_class=oracle.jdbc.OracleDriver
```

The previous value was:

```
hibernate.connection.driver_class=oracle.jdbc.driver.OracleDriver
```

11. Set IUCLID 5 to start in its update mode by uncommenting the following line in the file `server.properties`

```
database.update.startup=true
```

12. Start the IUCLID 5 server, and wait until the IUCLID database has been migrated. This can be followed from logs. During the migration, the IUCLID server status is *Unavailable*.

13. Stop the IUCLID 5 server.

14. Set IUCLID 5 to start not in its update mode by commenting out the line edited in step (11):

```
#database.update.startup=true
```

15. Start the IUCLID 5 server.

3.1.2. Starting IUCLID 5 after migration using the server method

If the migration process has been carried out successfully, you can now connect to the newly installed IUCLID in the same way as before the upgrade. The initialisation process is not required. All of the data that was present in the upgraded system should be present in the new system. Therefore, it should be possible to log in to any of the user accounts from the previous system.

3.2. Upgrading from IUCLID 5.0 or 5.1 to IUCLID 5.3

Important

There is no automatic upgrade of the database from IUCLID 5.0 / 5.1 to IUCLID 5.3. The data must be transferred manually from the old to the new database as described in the sub-section below.

Each installation of IUCLID 5 must have its own database and its own web application server. There can be more than one database running on a single instance of the database software, but each web application server cannot be used to run more than one IUCLID 5 application at once.

3.2.1. Migration of data to IUCLID 5.3 from IUCLID 5.0 or 5.1

Before starting to install IUCLID 5.3, all the data must be exported from IUCLID 5.1.x using the Back-up plugin that is available on the IUCLID web site. The export process is essential because the exported data will later be imported into IUCLID 5.3. When it is run, the Back-up plugin asks the user to create and enter a single password. This will become the password for all the user accounts in the new installation, with the exception of the account *SuperUser* which has a default password of *root*. To import the exported data into IUCLID 5.3, use the built-in Restore feature of IUCLID 5.3 that can be found from the menu File / Administrative tools. This feature allows the upload of data that was exported using the Back-up plugin on 5.1.x. Note that it is not possible to transfer data from either IUCLID 5.3 or IUCLID 5.2 to IUCLID 5.1.

3.2.2. Database configuration for running IUCLID 5.3 and a previous version at the same time

If you already have a previous version of IUCLID 5, it is recommended to keep it for the time being. It can be deleted in the future when you are absolutely sure that it is no longer needed. What follows is some information and advice as to how you can manage more than one version of IUCLID 5. As stated above, each installation of IUCLID 5 must have its own database and its own web application server. A new database must be created for IUCLID 5.3 because the structure of the database differs from that of previous versions. This requirement can be met in a variety of different ways. The following sub-sections describe some common sets of circumstances. The database for IUCLID 5.3 can be run on the same instance of the database software as a previous version of IUCLID 5, however, it must have a unique name within that instance of the database software. When IUCLID 5.3 is run for the first time on an empty database, it will automatically create all the correct tables.

3.2.2.1. If more than one computer is available for installation of IUCLID 5

Each instance of IUCLID 5 that is running in an application server is installed on a separate computer and has its own database. In this case, the instances of IUCLID 5 can point to databases that are either running on the same computers as the respective IUCLID 5s, or, on a central instance of the database software that contains a separate database for each of the instances of IUCLID 5. In all of these cases, each instance of IUCLID 5 is independent of all others such that a change to one is not reflected in any other. Data from an installation of IUCLID 5.1 can be transferred to an installation of IUCLID 5.3 using the Backup plugin in IUCLID 5.1 followed by use of the Restore feature in IUCLID 5.3. Note that it is not possible to transfer data from either IUCLID 5.3 or IUCLID 5.2 to IUCLID 5.1.

3.2.2.2. If only one computer is available for installation of IUCLID 5

If only one computer is available, only one web application server can be run at a once, and so only one instance of IUCLID 5 can be run at once. However, in this case, it is possible to have two different versions of IUCLID 5 installed on one computer, and to switch back and forth between them; running only one at a time. There are various different ways of doing that. What follows, is a description of one of the possible methods:

Before deploying an installation of IUCLID 5.3:

1. In IUCLID 5.1, install and run the Backup plugin.
2. In the Web Application Manager, make a note of the name of the path to the application (example: /iuclid51).
3. In the Web Application Manager, stop the IUCLID5 Server.
4. In the computer's file system, create a directory in which to store un-installed web applications (example: uninstalled_webapps).
5. In the computer's file system, copy the directory noted in step 1.2 (example: iuclid51) to the directory just created (example: uninstalled_webapps).
6. In the Web Application Manager, un-deploy the application (example: iuclid51).

Install IUCLID 5.3 as described in the installation manual. Note that a new database must be created. It can be running on the same instance of the database software, but in that case, the database must have a different name. When IUCLID 5.3 is running, use its built-in Restore feature to upload data from the back-up that was created during the initialisation process (step 1.1).

To switch between versions of IUCLID 5 (example: iuclid53 -> iuclid51)

1. In the Web Application Manager, make a note of the name of the path to the IUCLID 5 application from which you are switching (example: /iuclid53).
2. In the Web Application Manager, stop that IUCLID 5 application (example: iuclid53).
3. In the computer's file system, copy the application directory of the IUCLID 5 from which you are switching (example: iuclid53) to the directory *uninstalled_webapps*.
4. In the Web Application Manager, un-deploy the IUCLID 5 application from which you are switching (example: iuclid53).
5. In the computer's file system, move the directory of the IUCLID 5 to which you are switching (example: iuclid51); from the directory *uninstalled_webapps* to the directory *webapps*.
6. Start the IUCLID 5 application to which you are switching (example: iuclid51).

Before switching from IUCLID 5.1 to IUCLID 5.3, consider whether you would like to transfer data from 5.1 to 5.3. If you do want to transfer data, whilst you still have IUCLID 5.1 up and running, use the Back-up plugin to make a copy of your data. The copy can then be imported into IUCLID 5.3 using IUCLID 5.3's built-in Restore feature.

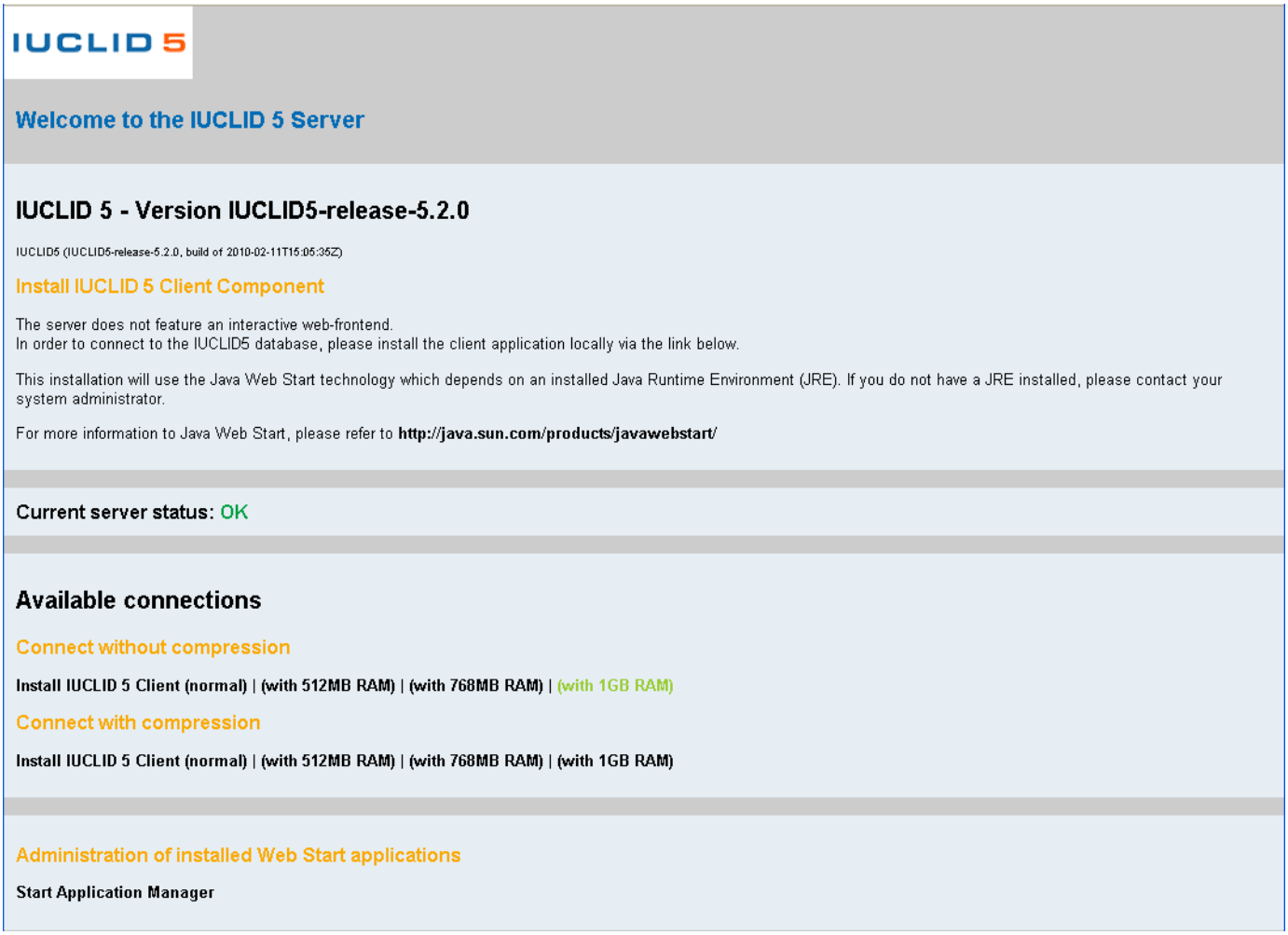
Chapter 4. Initialisation of an installation of IUCLID 5

This chapter describes the configuration that is required to create a working IUCLID 5 system from an installation of IUCLID 5 that has an empty database. There are two scenarios: either to create a working installation from scratch, or to load data from a back-up that was made using the built-in back-up function of IUCLID. During initialisation from scratch, reference substance data and a legal entity are uploaded into the database, and the required user accounts can be created. For initialisation from back-up, make sure that the back-up files are accessible from the system on which IUCLID will be initialised. What to do in each scenario is described in the rest of this chapter.

4.1. Starting IUCLID 5

Connect to the application with a browser by entering the address *http://<address of your server>:8080/i5server*. The following page is displayed.

Figure 4.1. The default page for Java Web Start of IUCLID 5


IUCLID 5
Welcome to the IUCLID 5 Server
IUCLID 5 - Version IUCLID5-release-5.2.0
IUCLID5 (IUCLID5-release-5.2.0, build of 2010-02-11T15:05:35Z)
Install IUCLID 5 Client Component
The server does not feature an interactive web-frontend.
In order to connect to the IUCLID5 database, please install the client application locally via the link below.
This installation will use the Java Web Start technology which depends on an installed Java Runtime Environment (JRE). If you do not have a JRE installed, please contact your system administrator.
For more information to Java Web Start, please refer to http://java.sun.com/products/javawebstart/
Current server status: OK
Available connections
Connect without compression
Install IUCLID 5 Client (normal) | (with 512MB RAM) | (with 768MB RAM) | (with 1GB RAM)
Connect with compression
Install IUCLID 5 Client (normal) | (with 512MB RAM) | (with 768MB RAM) | (with 1GB RAM)
Administration of installed Web Start applications
Start Application Manager

The page shown above page contains links that use Java Web Start technology to start a client that connects to the IUCLID server and displays IUCLID 5's graphical user interface (GUI) on the client machine. In the example shown above, the link under the text "IUCLID 5 Client (with 1GB RAM)" has already been followed. The difference between the links in the above

page is that each link passes different parameters to the IUCLID 5 server. The options included are for varying amounts of memory to be allocated to IUCLID 5 and for different types of data compression to be employed in the connection to the server. If IUCLID 5 runs slower than you would like and you have the available memory, select a link for a larger amount of RAM. The client can be run directly from a browser or by first downloading a file from one of the links and running that. Depending on your browser settings, when you click on one of the links above you will see either a dialogue box, or IUCLID 5 will run and you will see the login page. The browser dialogue asks whether you would like to save a file or run it straight away. The choice is yours. A convenient way to access IUCLID 5 is to download one of the files from the default page, save it to the desktop of your local machine used to access IUCLID 5 and give it the IUCLID 5 icon that comes with the installation. Double clicking on the icon then launches the IUCLID 5 GUI. Once you see the login page, you are ready to go walk through the First steps wizard, as described in the next section.

4.2. First steps wizard

When you start IUCLID 5 for the first time, the *First steps* wizard is run automatically. It guides you through the steps required to make a working user account and to upload the data required to use IUCLID 5 in a practical setting. The settings that relate to user accounts can also be changed after having run the wizard, using the features described in the IUCLID 5 User Manual.

Important

This wizard allows a single user account to be created, per run. This user is in addition to the *SuperUser* account that comes with the installation. It is essential to have at least one user account in addition to *SuperUser* because *SuperUser* should be used only for the special tasks that only it can carry out. See the IUCLID 5 User Manual for more detail.

As part of the First steps wizard, a legal entity must be uploaded into the IUCLID 5 installation in the form of a LEOX file. Therefore, before running this wizard, make sure that a LEOX file for the legal entity of your company or organisation is accessible to your computer. For more information, see the IUCLID 5 User Manual.

The First steps wizard provides the option of uploading the following information to your IUCLID 5 installation. For details, see the IUCLID 5 User Manual:

- EC Inventory
- Inventory of Reference substances

Although these uploads are optional, it is strongly recommended to do them during the first run of the First steps wizard. To do so, you will need to have the data accessible to your computer whilst running this wizard.

The First steps wizard can be run at any time, but only by the *SuperUser*. This is done from the file menu within IUCLID 5 **Administrative tools** / **Initialise**.

When starting the IUCLID 5 for the first time, the only user available is an administrator named *SuperUser*. Log in as *SuperUser* by entering the following case-sensitive values into the login screen as shown below:

Username: SuperUser

Password: root

The First steps wizard then proceeds. Each page of the wizard is described in a figure below.

Figure 4.2. Step 1 of the First steps wizard - Introduction

The wizard presents some useful information. There are no actions other than to read the information. Click the **Next** button.

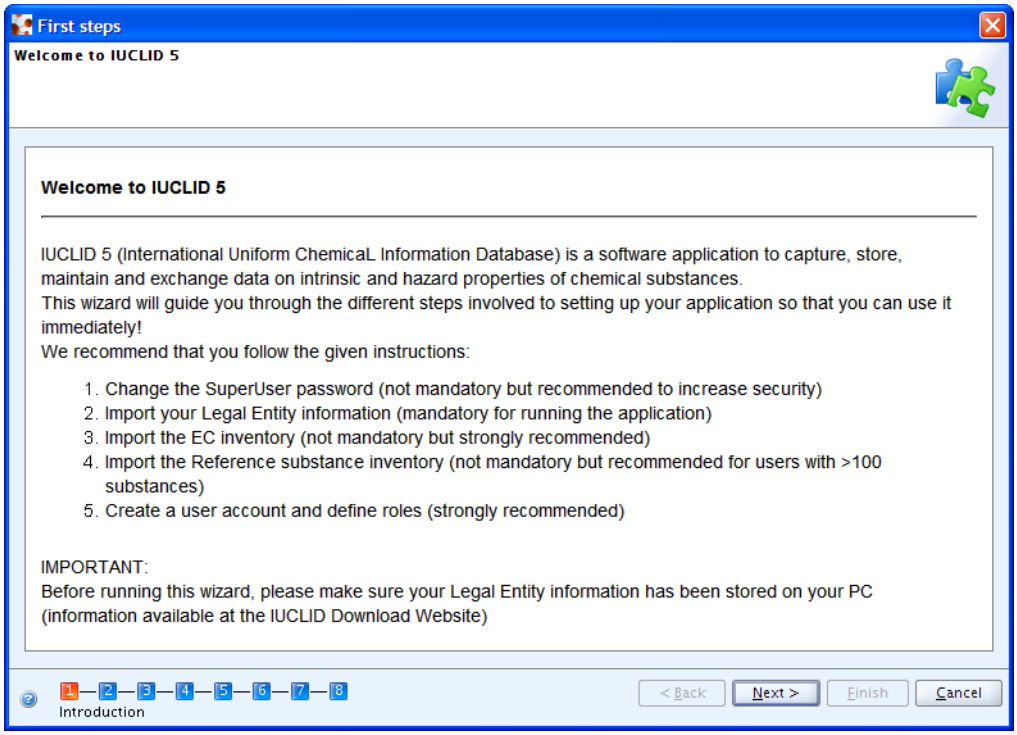

First steps
Welcome to IUCLID 5
Welcome to IUCLID 5
IUCLID 5 (International Uniform ChemicaL Information Database) is a software application to capture, store, maintain and exchange data on intrinsic and hazard properties of chemical substances.
This wizard will guide you through the different steps involved to setting up your application so that you can use it immediately!
We recommend that you follow the given instructions:
1. Change the SuperUser password (not mandatory but recommended to increase security)
2. Import your Legal Entity information (mandatory for running the application)
3. Import the EC inventory (not mandatory but strongly recommended)
4. Import the Reference substance inventory (not mandatory but recommended for users with >100 substances)
5. Create a user account and define roles (strongly recommended)
IMPORTANT:
Before running this wizard, please make sure your Legal Entity information has been stored on your PC (information available at the IUCLID Download Website)
1 2 3 4 5 6 7 8
Introduction
< Back
Next >
Finish
Cancel

Figure 4.3. Step 2 of the First steps wizard - Init mode - New installation

To initialise a new database, select the button `New Installation`as shown below and continue to the next step.

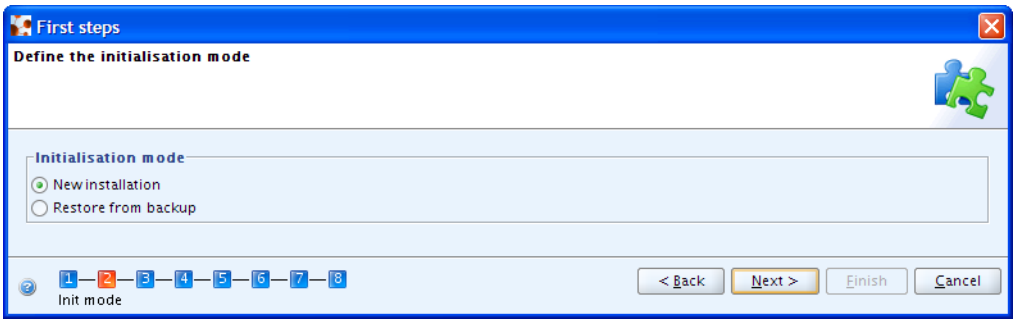
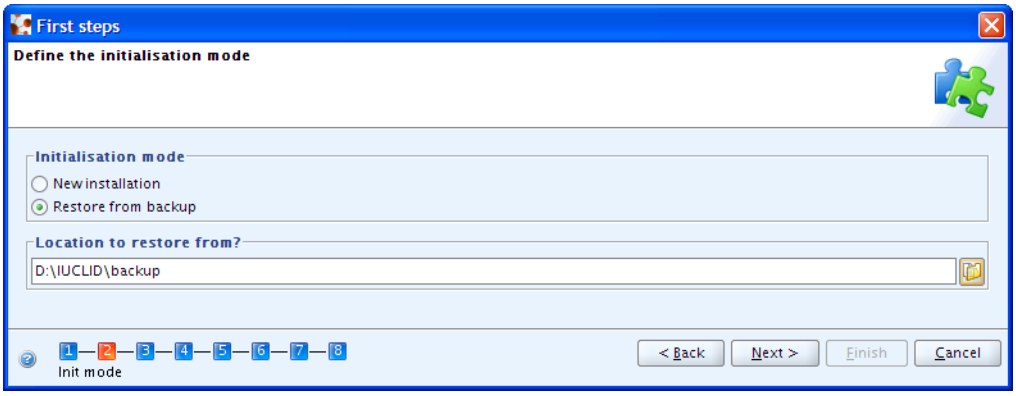


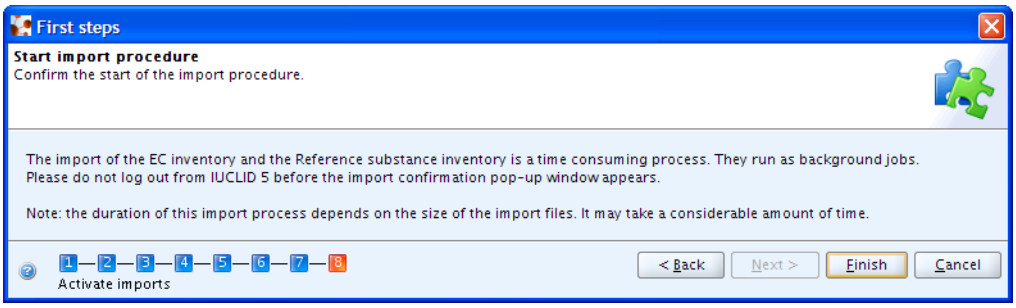
Figure 4.4. Step 2 of the First steps wizard - Init mode - Restore from backup

To restore from a backup of a previous version of IUCLID 5, select the button `Restore from backup` then enter the directory containing the backup files as shown in the example below.



Click **Next**. The wizard jumps to its last step, where the importation of data is started, as shown below.

Figure 4.5. Restoration from a back-up - Step 8 - Activate imports


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

The import may take some time. Click *Finish*. When the restoration is complete, the following screen is shown.

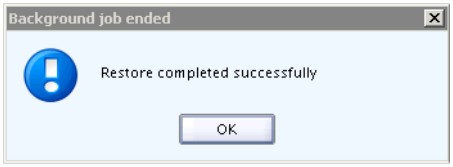


Figure 4.6. Step 3 of the First steps wizard - Change password

If you have not yet changed the default password of the *SuperUser* to a more secure value than *root*, the traffic light in the wizard screen will be yellow. To change the password, check the box `Change SuperUser password` , enter the old password *root* and then enter the new password. After confirming the password, click the button **Next**.

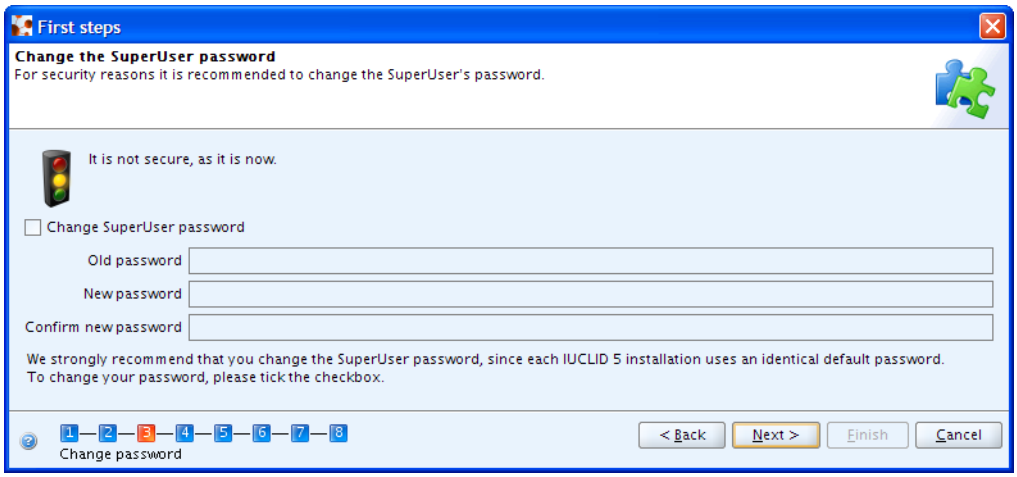
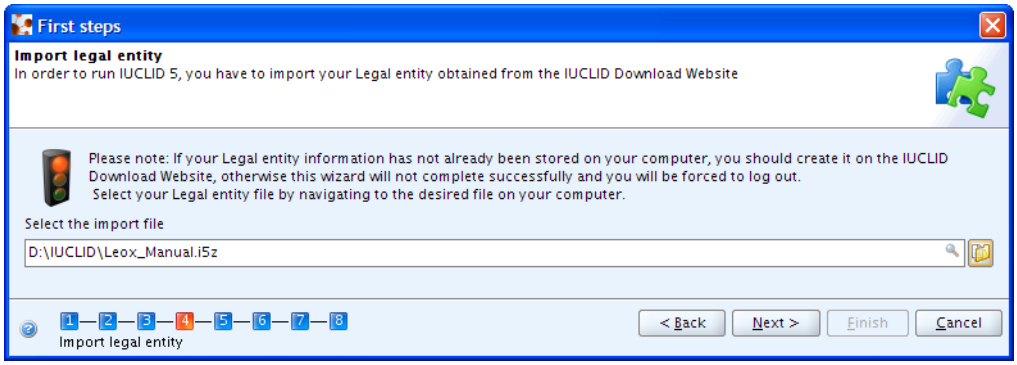
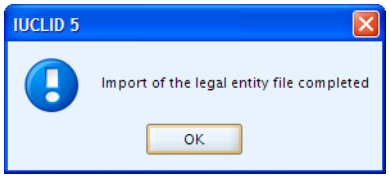

First steps
Change the SuperUser password
For security reasons it is recommended to change the SuperUser's password.
It is not secure, as it is now.
Change SuperUser password
Old password
New password
Confirm new password
We strongly recommend that you change the SuperUser password, since each IUCLID 5 installation uses an identical default password.
To change your password, please tick the checkbox.
1 2 3 4 5 6 7 8
Change password
< Back
Next >
Finish
Cancel

Figure 4.7. Step 4 of the First steps wizard - Import Legal Entity

To import a Legal entity (see the IUCLID 5 User Manual) select its LEOX file by browsing to the file. The browsing is accessed by clicking on the folder icon to the right of the field Select the import file. Click the **Next** button. The Legal entity is imported immediately.


First steps
Import legal entity
In order to run IUCLID 5, you have to import your Legal entity obtained from the IUCLID Download Website
Please note: If your Legal entity information has not already been stored on your computer, you should create it on the IUCLID Download Website, otherwise this wizard will not complete successfully and you will be forced to log out.
Select your Legal entity file by navigating to the desired file on your computer.
Select the import file
D:\IUCLID\Leox_Manual.i5z
1 2 3 4 5 6 7 8
Import legal entity
< Back
Next >
Finish
Cancel



Important

You must import at least one Legal entity in order to succeed with this wizard. If you have no Legal entity in the IUCLID 5 system, the traffic light in the wizard screen will be red. The First steps wizard will be automatically launched when you log in to IUCLID 5 until a Legal entity has been successfully imported.

Figure 4.8. Step 5 of the First steps wizard - Import EC Inventory

EC inventory import - To import the EC inventory, select the file for the EC inventory (see the IUCLID 5 User Manual). The EC Inventory will not be imported immediately. The import will start at the end of the First steps wizard. Depending on your machine speed and the size of the inventory, this import can take some time, e.g. up to half an hour.

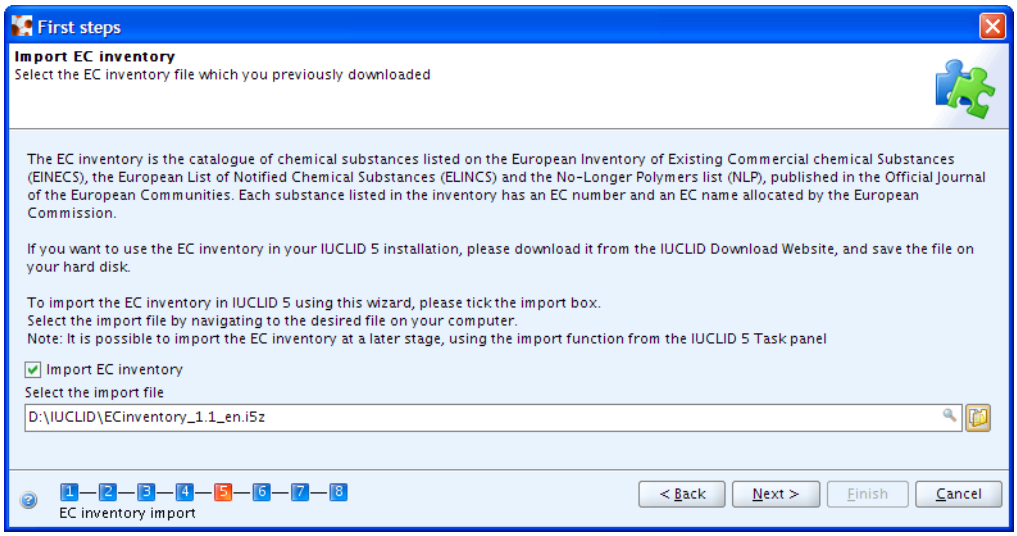
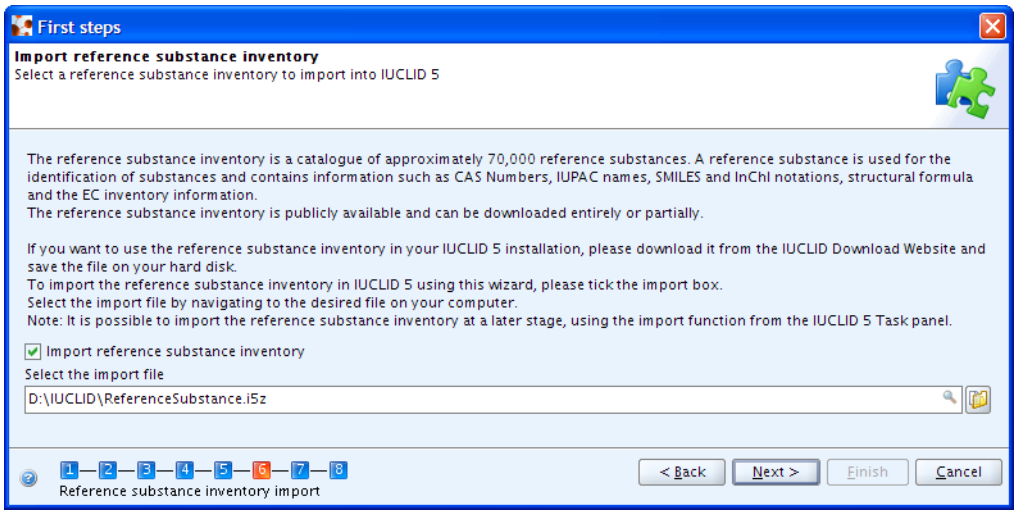

First steps
Import EC inventory
Select the EC inventory file which you previously downloaded
The EC inventory is the catalogue of chemical substances listed on the European Inventory of Existing Commercial chemical Substances (EINECS), the European List of Notified Chemical Substances (ELINCS) and the No-Longer Polymers list (NLP), published in the Official Journal of the European Communities. Each substance listed in the inventory has an EC number and an EC name allocated by the European Commission.
If you want to use the EC inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website, and save the file on your hard disk.
To import the EC inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the EC inventory at a later stage, using the import function from the IUCLID 5 Task panel
Import EC inventory
Select the import file
D:\IUCLID\ECinventory_1.1_en.i5z
1 2 3 4 5 6 7 8
EC inventory import
< Back
Next >
Finish
Cancel

Figure 4.9. Step 6 of the First steps wizard - Import reference substance inventory

Reference substance inventory import - Select the file for the Reference substance inventory (see the IUCLID 5 User Manual). The Reference substance inventory will not be imported immediately. The import will start at the end of the first steps wizard together with the EC Inventory import. Depending on your machine speed and the size of the inventory, this bulk operation may take a long time. The import of the Reference substance inventory itself can take **up to several hours**.

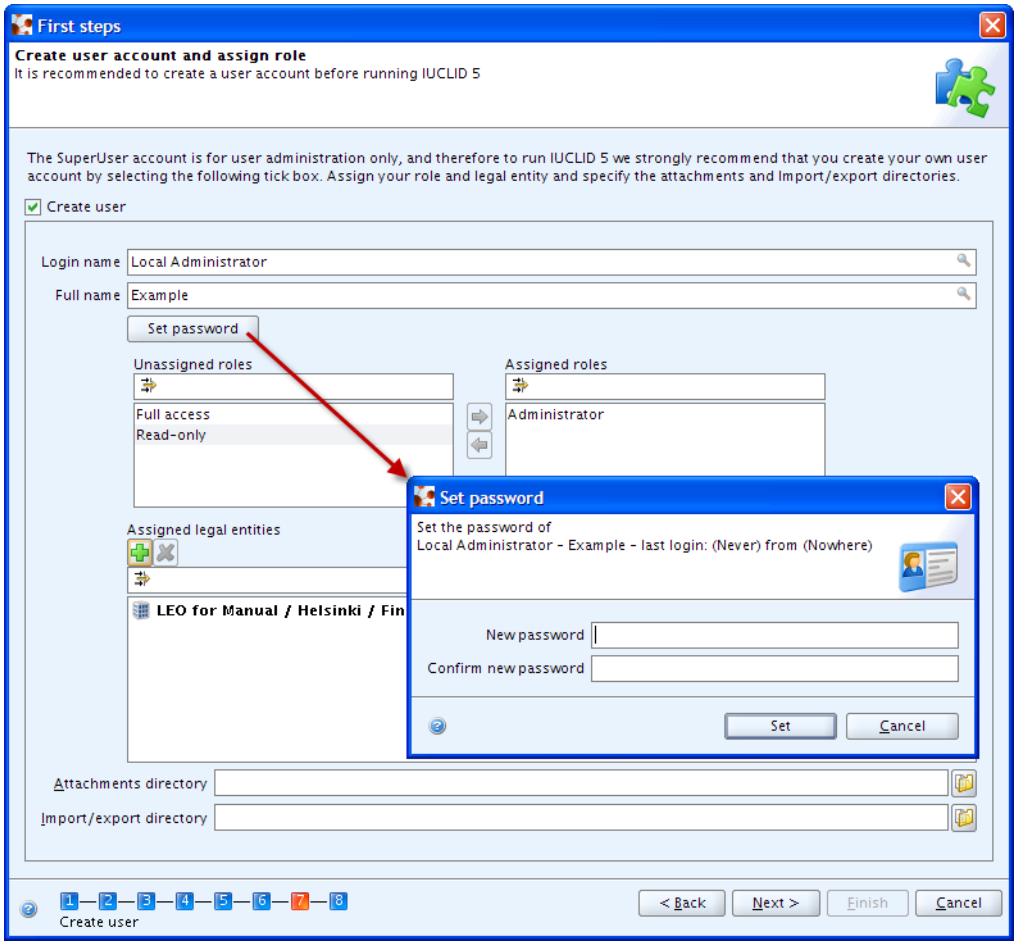

First steps
Import reference substance inventory
Select a reference substance inventory to import into IUCLID 5
The reference substance inventory is a catalogue of approximately 70,000 reference substances. A reference substance is used for the identification of substances and contains information such as CAS Numbers, IUPAC names, SMILES and InChI notations, structural formula and the EC inventory information.
The reference substance inventory is publicly available and can be downloaded entirely or partially.
If you want to use the reference substance inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website and save the file on your hard disk.
To import the reference substance inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the reference substance inventory at a later stage, using the import function from the IUCLID 5 Task panel.
Import reference substance inventory
Select the import file
D:\IUCLID\ReferenceSubstance.i5z
1 2 3 4 5 6 7 8
Reference substance inventory import
< Back
Next >
Finish
Cancel

Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set*, a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

Figure 4.10. Step 7 of the First steps wizard - Create user account and assign role

Create a new user account and define its user access rights by assigning it a role. It is essential to create a new user because general working within IUCLID 5 with the SuperUser is not supported. Only one user can be created per run of the First steps wizard.


First steps
Create user account and assign role
It is recommended to create a user account before running IUCLID 5
The SuperUser account is for user administration only, and therefore to run IUCLID 5 we strongly recommend that you create your own user account by selecting the following tick box. Assign your role and legal entity and specify the attachments and Import/export directories.
Create user
Login name
Local Administrator
Full name
Example
Set password
Unassigned roles
Full access
Read-only
Assigned roles
Administrator
Assigned legal entities
LEO for Manual / Helsinki / Fin
Set password
Set the password of
Local Administrator - Example - last login: (Never) from (Nowhere)
New password
Confirm new password
Set
Cancel
Attachments directory
Import/export directory
1 2 3 4 5 6 7 8
Create user
< Back
Next >
Finish
Cancel

- Select the checkbox `Create user`.

  Fill in all the fields. The user needs a `Login name` for identification during login. The `Full name` is used for proper user identification. The `Assigned role` is needed to administrate the access permissions. In a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default.

- Enter a `Login name`, as it should be used for identification during login, and the `Full name` used for proper user identification.

- Optionally, click Set password and define a password.

- Click and highlight a role in the list of unassigned roles and assign it to the user by clicking the Right arrow. Assigning a Role is needed to administrate the access permissions (in a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default).

Tip

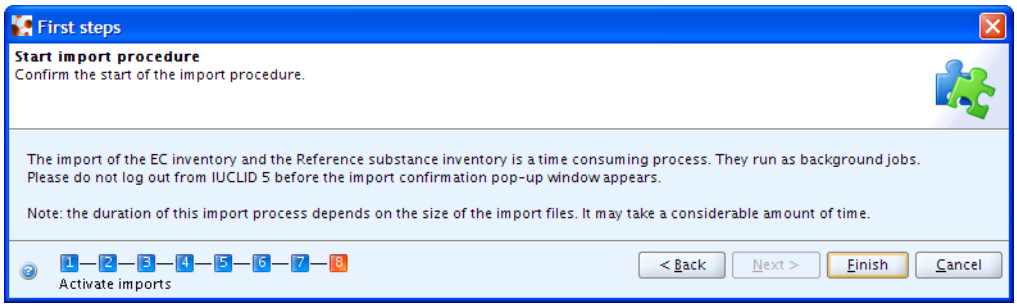
It is recommended to create a user with the *Administrator* Role regardless of whether a stand alone or a distributed version of IUCLID 5 is set up. Once a user has been created, the IUCLID 5 administrator (in case of a distributed version) can define different other user(s) and assign different role(s) to them (see the IUCLID 5 User Manual).

- Assign a Legal entity (normally the Legal entity imported in the third step of this wizard) by clicking the green plus button and performing a search for the desired Legal entity. In the Query field `Legal entity name`, enter the name of the desired Legal entity or an asterisk (*) as wildcard and click the **Search** button. In the Query results list, click the desired entry and then click the **Assign** button.
- Optionally, select default attachment and import/export directories. These settings can be changed at a later stage, as described in the IUCLID 5 User Manual.
- Click the **Next** button

Figure 4.11. Step 8 of the First steps wizard - Start import procedure

If you have selected an EC Inventory and/or Reference substances inventory file(s) during the wizard steps, you can now run the imports. Click the button **Execute imports**. Note again that these imports can take up to several hours, depending on your machine speed and the amount of data you are importing.

Then click the button **Finish**. If you have launched any imports, you will now have to wait until the imports are completed. Afterwards, you should log out and then log in again as a user for the newly defined account. Remember: general working as SuperUser is not supported.


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

4.3. User management

The installation of IUCLID 5 is now ready for hand-over to whoever will be maintaining the system and whoever will be managing the user accounts. The management of user accounts and their roles is described in the IUCLID 5 User Manual. Individual users can connect to the IUCLID 5 server using Java Web Start technology, as described in section 3.1 of this document. A convenient way to achieve that is for users to save onto their desktop, one of the files downloaded from the default Java Web Start page. The user would launch IUCLID 5 by simply double-clicking on the icon on his or her desktop. Alternatively, the users could be supplied with the URL *http://<address of your server>:8080/i5server* and instructions on which link to use.

Chapter 5. Un-installation of IUCLID 5

The un-installation of IUCLID is a manual process. IUCLID can be un-installed by deleting the files that were copied to the destination machine, and reversing any changes made during the installation process. For more details about the actions that might be required, see the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.